

# **Simulations of Transient Fuel Gases Mixing in Air**

by

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JANUARY 2014

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## **CERTIFICATION OF APPROVAL**

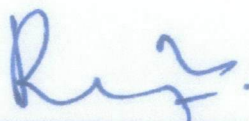
### **SIMULATIONS OF TRANSIENT FUEL GASES MIXING IN AIR**

by

**Irsyad Ahnaf Bin Azman**

A project dissertation submitted to the  
Chemical Engineering Programme  
Universiti Teknologi PETRONAS  
in partial fulfillment of the requirement for the  
**BACHELOR OF ENGINEERING (Hons)**  
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**TRONOH, PERAK**  
**SEPTEMBER 2013**

## CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

A handwritten signature in blue ink, appearing to read 'Irsyad Ahnaf Bin Azman', written over a horizontal line.

IRSYAD AHNAF BIN AZMAN

## **ABSTRACT**

The lack of fundamental understanding about the dispersion of fuel gases after leakage occurrence has encouraged this project to be done. The objective of this project is to study the behavior of fuel gases when it mixed with air in 2D simulation. This project also aims to study the formation and decomposition of flammability region when fuel gases mixed with air. The problems with fuel gases are that most of them are almost untraceable. Most of them are odorless and colorless. Should any leaks occur, it is very hazardous. This project will be very useful in developing fuel gases detection system. The fuel gases that were accounted are methane, hydrogen, ethane, propane, butane, carbon monoxide and acetylene. Computational Fluid Dynamics (CFD) simulation is use in this project as tools to study the behavior of transient mixing of fuel gases with air and the development and decay of flammability region. The expected results are as the picture below.



## **ACKNOWLEDGEMENT**

The author would like to express deepest gratitude towards the Chemical Engineering Department of Universiti Teknologi PETRONAS for providing the software and also for the permission to use Blok 5 Simulation Lab. My gratitude also goes to Dr Rajashekhar Pendyala for guiding me in completing this project. Last but not least to FYP Coordinator and all FYP Examiners. This project has turned out to be a successful and meaningful paper for fundamental research understanding of transient fuel gas dispersion.

## TABLE OF CONTENTS

|  |      |
|--|------|
| CERTIFICATION OF APPROVAL .....              | ii   |
| CERTIFICATION OF ORIGINALITY .....           | iii  |
| ABSTRACT.....                                | iv   |
| ACKNOWLEDGEMENTS .....                       | v    |
| TABLE OF CONTENTS.....                       | vi   |
| LIST OF FIGURES .....                        | viii |
| LIST OF TABLES .....                         | ix   |
| <br>   |      |
| CHAPTER 1: INTRODUCTION.....                 | 1    |
| 1.1 Background Study.....                    | 1    |
| 1.2 Problem Statement .....                  | 2    |
| 1.3 Objectives .....                         | 2    |
| 1.4 Scope of Study .....                     | 2    |
| 1.5 Relevancy of the Project.....            | 3    |
| 1.6 Project Feasibility.....                 | 3    |
| <br>   |      |
| CHAPTER 2: LITERATURE REVIEW .....           | 4    |
| <br>   |      |
| CHAPTER 3: RESEARCH METHODOLOGY .....        | 10   |
| 3.1 Work Flow Process .....                  | 10   |
| 3.1.1 Pre-analysis & Geometry Modeling ..... | 11   |
| 3.1.2 Meshing.....                           | 12   |
| 3.1.3 Setup Physics.....                     | 13   |
| 3.1.4 Solution .....                         | 16   |
| 3.1.5 Result .....                           | 16   |
| 3.1.6 Verification & Validation .....        | 17   |
| 3.2 Gant Chart.....                          | 18   |
| 3.3 Simulation Tool.....                     | 19   |

**CHAPTER 4: RESULT AND DISCUSSION .....20**

    4.1 Dispersion Behavior of Fuel Gases in Enclosed Geometry .....20

    4.2 Formation of Flammability Region.....28

    4.3 Comparison of Open Top Geometry and Enclosed Geometry .....36

**CHAPTER 5: CONCLUSION AND RECOMMENDATION .....38**

**REFERENCES.....40**

## LIST OF FIGURES

|                 |  |    |
|-----------------|--|----|
| Figure 1.1:     | Proposed Geometry Setting .....  | 3  |
| Figure 2.1:     | Geometry Setting .....   | 6  |
| Figure 2.2:     | Display of formation of flammability region for hydrogen using ANSYS software. ....                                | 9  |
| Figure 3.1:     | ANSYS method of simulation .....   | 10 |
| Figure 3.2:     | Uniform Meshing and Non-Uniform Meshing .....  | 12 |
| Figure 3.3:     | General Setup .....  | 13 |
| Figure 3.4:     | Energy Equation Setting.....   | 14 |
| Figure 3.5:     | Laminar Flow Setting.....  | 14 |
| Figure 3.6:     | Species Model Setting.....   | 15 |
| Figure 3.7:     | Expected Initial Graphic.....  | 16 |
| Figure 3.8:     | Desired Result.....  | 17 |
| Figure 4.1 (a): | Dispersion Behavior of Fuel Gases.....   | 21 |
| Figure 4.1 (b): | Dispersion Behavior of Fuel Gases .....  | 22 |
| Figure 4.2:     | Graph of Mole Fraction of $H_2$ vs. Position along centre of Geometry .....  | 24 |
| Figure 4.3:     | Graph of Mole Fraction of $CH_4$ vs. Position along centre of Geometry.....  | 25 |
| Figure 4.4:     | Graph of Mole Fraction of $C_2H_2$ vs. Position along centre of Geometry .....                                     | 26 |
| Figure 4.5:     | Graph of Mole Fraction of $CO$ vs. Position along centre of Geometry .....   | 27 |
| Figure 4.6:     | Formation of Flammability Region for Hydrogen.....   | 29 |
| Figure 4.7:     | Formation of Flammability Region for Methane .....   | 30 |
| Figure 4.8:     | Formation of Flammability Region for Acetylene .....   | 31 |
| Figure 4.9:     | Formation of Flammability Region for Carbon Monoxide .....   | 32 |
| Figure 4.10:    | Formation of Flammability Region for Ethane .....  | 33 |
| Figure 4.11:    | Formation of Flammability Region for Propane .....   | 34 |
| Figure 4.12:    | Formation of Flammability Region for Butane .....  | 35 |
| Figure 4.13:    | Comparison of dispersion behavior of hydrogen between open top geometry (left) and enclosed geometry (right) ..... | 36 |
| Figure 4.14:    | Comparison of dispersion behavior of methane between open top geometry (left) and enclosed geometry (right) .....  | 37 |

**LIST OF TABLES**

Table 2.1: Densities, Molecular Weight and Chemical Formulas .....5

Table 2.2: Lower Flammability Limit and Upper Flammability Limit of Fuel Gases .....8

Table 4.1: Density Comparison.....23

Table 4.2: Time Taken to Reach Top of Geometry.....28

Table 4.3: Range of Flammability Region.....29



# **CHAPTER 1**

## **INTRODUCTION**

### **1.1 Background Study**

Nowadays, the world's demand for energy is increasing year by year. In the year 2007, 86 million barrels of oil was consumed per day in average and it is expected to increase to 89.7 million barrels per day in 2013 ([gaspricesexplained.org](http://gaspricesexplained.org)). One source of energy is the fuel gases. Fuel Gases usually used with oxygen for heating purposes. Examples of fuel gases are natural gas, methane, ethane, hydrogen, propane and acetylene.

In order to accommodate the high demand of energy, production of fuel gases at all stages must be carried out efficiently, effectively and safely. All safety issues in upstream production, transportation and processing of fuel gases must be address thoroughly. Fuel gases pose an unseen threat because of its two physical properties that is colorless and odorless. A small leakage along pipelines or in plant can cause fire or even worse a fatal explosion. A gas leaks refer refers to a leak of leak of fuel gases from a pipe or containment, into living area or any other area that the gas should not be.

Transient mixing of fuel gas with air have not been studied comprehensively. It is hard to determine the formation and decay of flammable zones by experiments and theoretical hand calculations (Zhang, 2009). With the help of Computational Fluid Dynamic (CFD) and ANSYS Fluent Software, the numerical simulation displays of the spatial and temporal distributions of fuel gas for all configurations can be studied.

As a conclusion, the complex flow patterns demonstrate the fast formation of flammable zones with implications in the safety management and efficient use of fuel gases in various applications.

## **1.2 Problem Statement**

Two physical properties of fuel gases are odorless and colorless. The fact that the fuel gases pose these properties makes them hazardous should any leak occur. If any leaks occur, the fuel gas can accumulate and may lead to fire or even worse, an explosion. Poor understanding of the dynamic properties of fuel gases may lead to unawareness about fuel gas leaks. This project will be significant for developing fuel gas sensor system and also will be useful for concentration mapping in a plant or where fuel gases is utilize. In a nutshell, it is vital for dispersion pattern of fuel gas and formation of flammability envelope to be studied.

## **1.3 Objectives**

1. To develop and study the pattern of transient dispersion behavior of fuel gases when mixed with air in 2D simulation.
2. To develop and study the development and decay of flammability zones when mixed with air.

## **1.4 Scope of Study**

The project will cover the study of transient dispersion and flammability limits of the following fuel gas:

- 1) Methane
- 2) Hydrogen
- 3) Ethane
- 4) Propane
- 5) Butane
- 6) Carbon Monoxide
- 7) Acetylene

2D simulation of ANSYS Fluent 14.0 software will be use to obtain the final result which is the display of fuel gases mixing with air and respective flammability limits of fuel gas in air. The following geometry setup will be use:

1. Initial 10% of fuel gas at the bottom and 90% air at the top of the geometry in a closed geometry.
2. Initial 10% of fuel gas at the bottom and 90% air at the top of the geometry in an open top geometry.

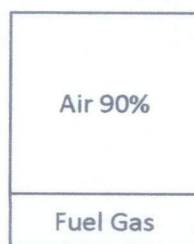


Figure 1.1: Proposed Geometry Setting

### 1.5 Relevancy of the Project

This project will be relevance for developing mitigation plan in safety management where fuel gases are involved. It will be useful for fuel gases detection system in plant or anywhere that involved the usage of fuel gases. In order to improve the process safety and loss prevention, the behavior of these gases when mixed with air should be understood.

### 1.6 Project Feasibility

With the time frame given of two semester or 8 months, this project can be completed. In fact it is expected for this project to be completed early because there is less work to be done since we use CFD simulation.



## **CHAPTER 2**

### **LITERATURE REVIEW**

In this project, we are studying the behavior of various fuel gases when it mixed with air. Development and decomposition of flammable region are difficult to predict by experiments (Shravan and Umit, 2009). As an alternative, Computational Fluid Dynamic (CFD) Software was used in order to understand the behavior of fuel gases and the formation of flammability limit when mixed with air. CFD is a systematic application of computational solution technique to mathematical models formulated to describe and simulate fluid dynamic phenomena ([web.cos.gmu.edu](http://web.cos.gmu.edu)). CFD is the best method to study instantaneous dispersion of natural gas (Yuanpan, et al.). In addition of that, running a CFD simulation is definitely easier, cheaper and more advantageous compared to do experiments. It is because of the accurate prediction of development and decomposition of flammable zones that the simulation software will provide if compared to experiments and theoretical hand calculation (Zhang, et al, 2007). To further deepen our research about the fuel gases behavior, we planned to do 3D simulation instead of just 2D simulation. CFD simulation can realize three-dimensional simulation and provide dynamic simulation of the whole process of heavy gas dispersion (Yuanpan, et al.).

Each Density of fuel gases are compared with air density of 1.205 kg/m<sup>3</sup> at standard conditions. Quicker dispersion of a lower density fuel gases are predicted. This prediction is base on a simple concept of that the lighter fuel gas will be quicker to the top and the heavier gas will be more likely to stay at the bottom.

Table 2.1: Densities, Molecular Weight and Chemical Formulas (Develop from engineeringtoolbox.com)

| Fuel Gases         | Density<br>(kg/m <sup>3</sup> ) | Molecular<br>Weight | Comparison with<br>Density of Air<br>(1.205 kg/m <sup>3</sup> ) | Chemical<br>Formula            |
|--------------------|---------------------------------|---------------------|---|--------------------------------|
| Methane            | 0.668                           | 16.043              | Less Dense  | CH <sub>4</sub>                |
| Hydrogen           | 0.0899                          | 2.016               | Less Dense  | H <sub>2</sub>                 |
| Ethane             | 1.264                           | 30.07               | More Dense  | C <sub>2</sub> H <sub>6</sub>  |
| Propane            | 1.882                           | 44.09               | More Dense  | C <sub>3</sub> H <sub>8</sub>  |
| Butane             | 2.489                           | 58.1                | More Dense  | C <sub>4</sub> H <sub>10</sub> |
| Acetylene          | 1.092                           | 26                  | Less Dense  | C <sub>2</sub> H <sub>2</sub>  |
| Carbon<br>Monoxide | 0.0727                          | 28.01               | Less Dense  | CO                             |

The first step in using any CFD simulation is to create a basic geometry for the simulations. A simple geometry of a 1 meter height cylinder with a 0.25 meter diameter was chosen to be the geometry in CFD simulations (Shravan and Umit, 2009). Next step is to specify the composition inside the geometry. The composition inside the geometry at time = 0s is 10% hydrogen at the bottom with air filling the rest upper part of the geometry (refer figure 2). Three different cases that were studied were completely open top cylinder, partially open top cylinder and fully closed top cylinder. The existing models should be modified to predict confined vented and unconfined vapor cloud involving natural gas (Mumby, 2010).

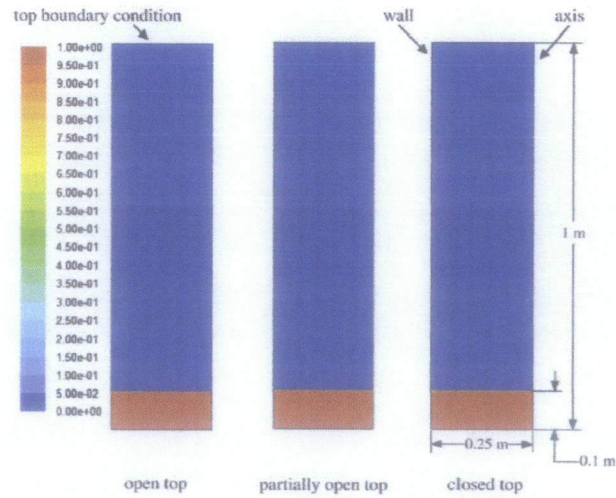


Figure 2.1: Geometry Setting (Shravan K. Vudumu & Umit O. Koylu, 2009)

After the geometry has been fixed, the next step is the meshing step. Since hydrogen has high diffusive nature, a fine mesh with the minimum size of 0.1mm must be used. The time interval should also be very small to accommodate the hydrogen diffusive nature (0.001s). In order to achieve convergence, 50 iterations are performed at each time interval. Stationary, no slip and adiabatic wall boundary conditions are applied on the walls of the cylinder (Shravan and Umit, 2009).



In order to express the fluid movement, navier stokes equation alongside others necessary equations are use. The Navier-stokes equations assume that the fluid being studied is a continuum (it is infinitely divisible and not composed of particles such as atoms or molecules), and is not moving at relativistic velocities (Fluid Mechanics MCGraw-Hill, 2008).

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v}\right) = -\nabla p + \mu \nabla^2 \vec{v} + \vec{f}$$

Other than the navier-stokes equations, equations for conservation of mass, momentum, energy and mass diffusion are considered (Shravan K. Vudumu & Umit O. Koylu, 2009).

Mass Conservation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0$$

Momentum Equation

$$\frac{\partial}{\partial t}(\rho \vec{V}) + \nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla p + \nabla \cdot (\vec{\tau}) + \rho \vec{g}$$

Where  $\vec{\tau} = \mu[(\nabla \vec{V} + \nabla \vec{V}^T) - (2/3)\nabla \cdot \vec{V}]$  is the stress tensor.

Energy Conservation

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{V}(\rho E + p)) = \nabla \cdot (\kappa \nabla T - \sum_j h_j \vec{J}_j + (\vec{\tau} \cdot \vec{V})) + \rho(\vec{V} \cdot \vec{g})$$

Where  $E = h - (p/\rho) + (V^2/2)$  and  $h = \sum_j Y_j h_j$

Mass Diffusion

$$\vec{J}_i = -\rho D_i \nabla Y_i$$

Flammability limit is the amount of combustible gas in an air mixture when the mixture is flammable. Fuel gases are only flammable under certain conditions. The lower flammability limit (LFL) shows the minimum fuel concentration to sustain a flame and the upper flammability limit (UFL) shows the maximum fuel concentration to starts a fire. The LFL and UFL usually expressed as volume percent fuel (% of fuel + air) at atmospheric temperature and pressure. (Daniel and Joseph)

Table 2.2: Lower Flammability Limit and Upper Flammability Limit of Fuel Gases  
(Develop from [www.sensidynegasdetection.com](http://www.sensidynegasdetection.com))

| Fuel Gases      | LFL in %         | UFL in %         |
|-----------------|------------------|------------------|
|                 | By volume of air | By volume of air |
| Methane         | 4.4 - 5          | 15 - 17          |
| Hydrogen        | 4                | 75               |
| Ethane          | 3                | 12 - 12.4        |
| Propane         | 2.1              | 9.5 – 10.1       |
| Butane          | 1.6              | 8.4              |
| Acetylene       | 2.5              | 82               |
| Carbon Monoxide | 12               | 75               |

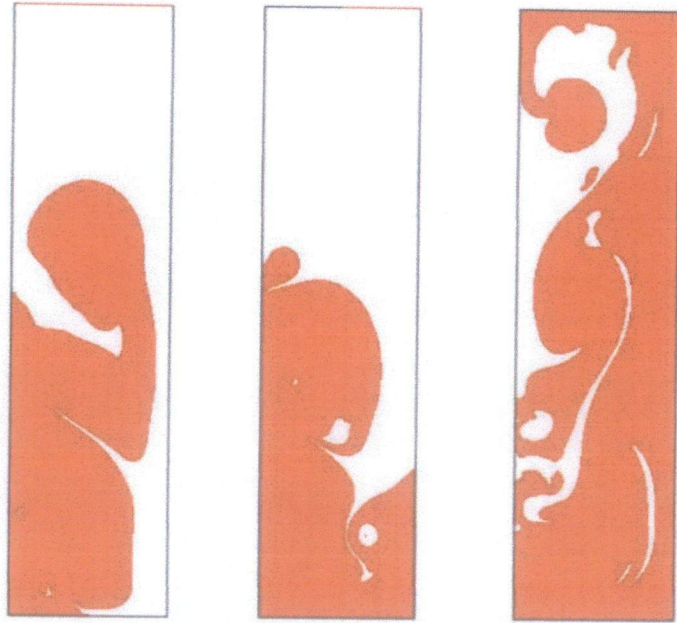


Figure 2.2: Display of formation of flammability region for hydrogen using ANSYS software (Shravan and Umit, 2009)

## CHAPTER 3

### RESEARCH METHODOLOGY

#### 3.1 Work Process Flow

In this project, Computational Fluid Dynamics (CFD) simulation is used to study the behavior of transient mixing of fuel gases with air and the development and decay of flammability region. The geometry is created and meshed in ANSYS 12.1 which is the preprocessor for FLUENT. First of all, geometry needs to be created in geometry steps. For this project, a simple vertical cylinder is being taken as our geometry. Next, the geometry needs to be meshed to divide the geometry into many parts. In the setup physics part, the boundary conditions and the specific conditions in the geometry are specified. Then come the solution part where we specified the method for the software to calculate the result for us and last but not least the result part where we extract the result in form of graph or displays.

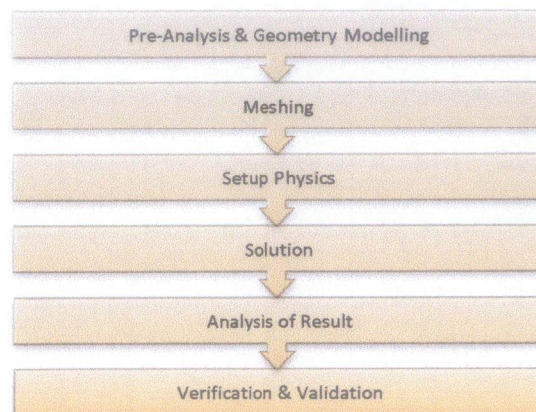
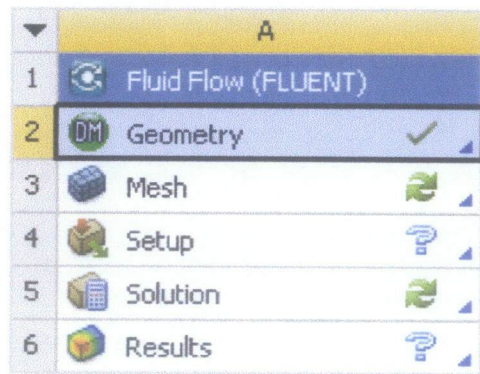


Figure 3.1: ANSYS method of simulation









### 3.1.1 Pre-analysis & Geometry Modeling



The first step in doing simulation is to decide the geometry. In this part, we can decide the geometry to be in 2 dimensional (2D) and 3 dimensional (3D). In this project, a 2D and 3D vertical cylinder with the dimension 1m height and 0.25m diameter need to be created. In this part also we need to specify the name for each side of the geometry. Next step is to create the surface body for the object. The constructed geometry can be transported into ANSYS Fluent for further meshing.



3.1.2 Meshing

|   |   |                     |   |
|---|---|---------------------|---|
| ▼ | A   |                     |   |
| 1 |  | Fluid Flow (FLUENT) |   |
| 2 |  | Geometry            | ✓ |
| 3 |  | Mesh                | ✓ |
| 4 |  | Setup               | ↻ |
| 5 |  | Solution            | ? |
| 6 |  | Results             | ? |

In meshing step, we decide how our mesh of geometry will be. Meshing will divide the area into parts where the calculations takes places and it is very important in order to obtain more accurate results. Non-uniform meshing has more coverage points compared to uniform meshing. The difference can be illustrated by the picture below.

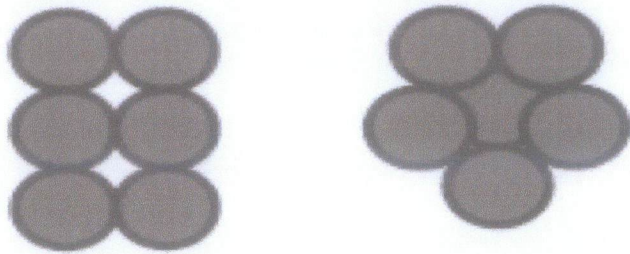


Figure 3.2: Uniform Meshing and Non-Uniform Meshing

Non-uniform meshing is more suitable to be located at the point where the diffusion of fuel gases occur and the uniform meshing is favored near wall boundary. In this project a really fine mesh will be needed. This is because of the highly diffusive nature of fuel gases in air. A minimum size of 0.1mm size of element should be used.

### 3.1.3 Setup Physics

After meshing, the next step is to specify the general setup for the simulation. Conditions such as the type of fluid, temperature, density, type of flow, viscosity, and boundary condition will be set. In this project, 7 different flue gases will be studied. We also need to specify the initial composition inside the geometry which is 10% of fuel gases and 90% of air. First the general setup has to be specified. For solver, we choose pressure based, absolute velocity formulation, transient, 2D planar and gravitational force acting in downwards direction.

The image shows the 'General' setup window in ANSYS Fluent. It is divided into several sections: 'Mesh' with buttons for 'Scale...', 'Check', 'Report Quality', and 'Display...'; 'Solver' with radio buttons for 'Type' (Pressure-Based selected, Density-Based unselected), 'Velocity Formulation' (Absolute selected, Relative unselected), 'Time' (Steady unselected, Transient selected), and '2D Space' (Planar selected, Axisymmetric unselected, Axisymmetric Swirl unselected); a checked 'Gravity' checkbox with a 'Units...' button; and 'Gravitational Acceleration' with input fields for X (m/s<sup>2</sup>) set to 0, Y (m/s<sup>2</sup>) set to -9.81, and Z (m/s<sup>2</sup>) set to 0.

Figure 3.3: General Setup

Model setup in this project will include energy equation, laminar flow model and species transport model. We specify the energy the usage of energy equation or not by ticking the box as shown below.

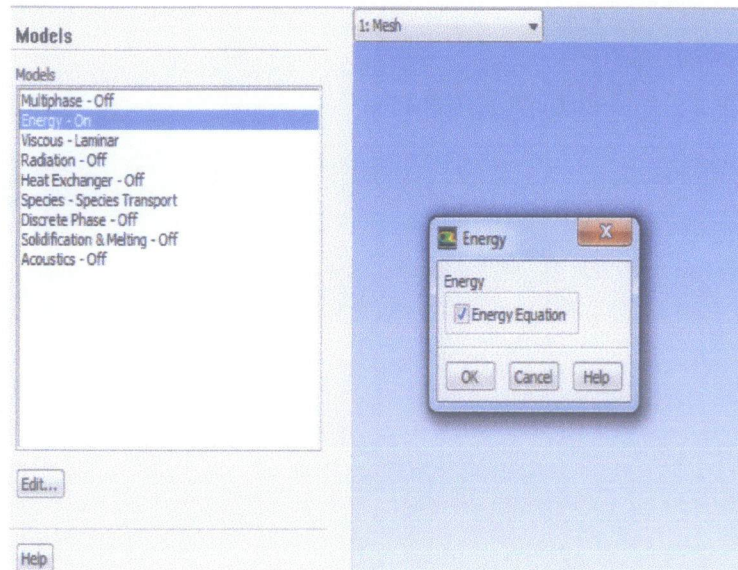


Figure 3.4: Energy Equation Setting

Laminar flow model is specified by double clicking on “viscous” and the laminar type of flow is chosen.

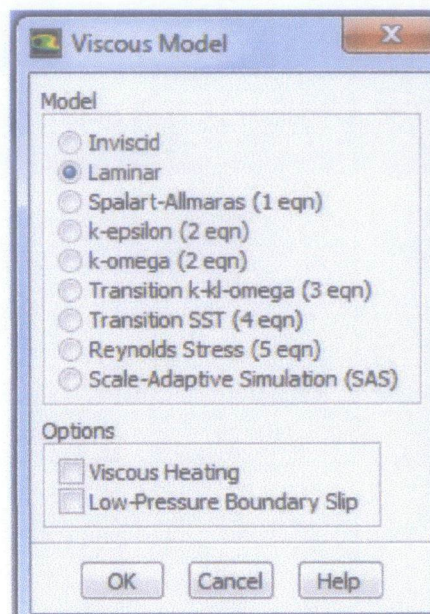


Figure 3.5: Laminar Flow Setting



The species model inside the geometry can be specified for instance, hydrogen-air is specified to indicate that hydrogen and air will be inside the geometry.

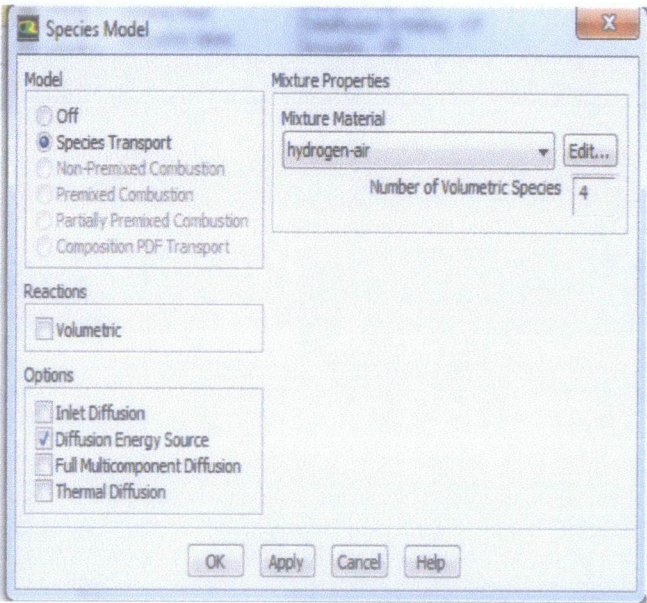


Figure 3.6: Species Model Setting

After that, we must specify the boundary conditions. In this project, the wall boundary is stationary and non-slip condition is chosen. The next step is to performed solution initialization where we specify the initial value of air. Here we key in 0.27 for  $O_2$  and 0.79 for  $N_2$  air is composed of 21% of oxygen and 79% of nitrogen. The geometry is now initially filled with air and to add the fuel gases, a method called “patching” is done. The expected graphics after initialization is as below.

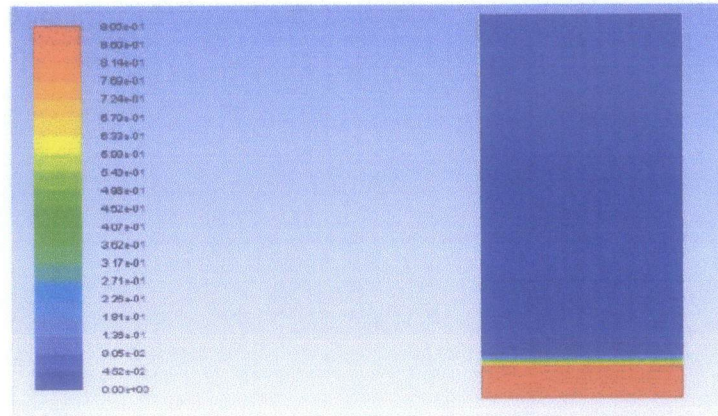


Figure 3.7: Expected Initial Graphic

### 3.1.4 Solution

This part is focusing more on how we will setup the software to calculation our result. The algorithm chosen in our calculation is SIMPLE algorithm. SIMPLE stand for Semi-Implicit Method for Pressure Linked Equations and it is commonly used to solve the Navier-stoke equations. We use *second order implicit* for unsteady flow equations for better accuracy. 0.01s is set to be the time step so that the simulation will be captured every 1 second and 50 numbers of iterations is chosen.

### 3.1.5 Result

This part will be the part where we will specify the software to produce the displays that we want. In this project, the result that we want is the display of behavior of transient mixing of fuel gases with air and the display of flammability envelope. The desired outcome can be seen from the picture below.

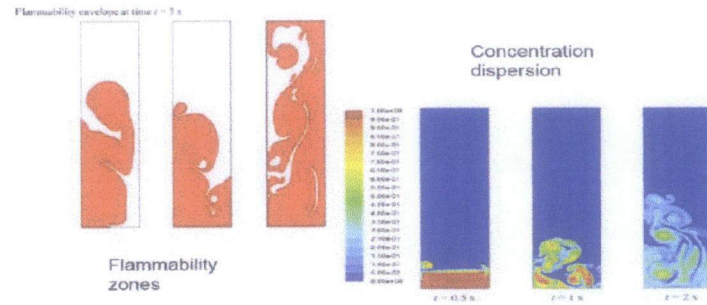


Figure 3.8: Desired Result

Animations may also be recorded to observe the mixing behavior.

### 3.1.6 Verification & Validation

Based on initial prediction which is using density differences, we will know that hydrogen will move to the top fastest compared to the other fuel gases. From our result later, comprehensive studied will be carried out to verify the hypothesis.

3.2 Gant Chart

Final Year Project 1

| Project Activities                 | Week |   |   |   |   |   |   |   |   |    |    |    |    |    |
|------------------------------------|------|---|---|---|---|---|---|---|---|----|----|----|----|----|
|                                    | 1    | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
| Project Draft                      |      |   |   |   |   |   |   |   |   |    |    |    |    |    |
| ANSYS Tutorial                     |      |   |   |   |   |   |   |   |   |    |    |    |    |    |
| Extended Proposal Preparation      |      |   |   |   |   |   |   |   |   |    |    |    |    |    |
| Extended Proposal Submission       |      |   |   |   |   |   |   |   |   |    |    |    |    |    |
| Proposal Defense                   |      |   |   |   |   |   |   |   |   |    |    |    |    |    |
| Project Work                       |      |   |   |   |   |   |   |   |   |    |    |    |    |    |
| Submission of Interim Draft Report |      |   |   |   |   |   |   |   |   |    |    |    |    |    |
| Submission of Interim Report       |      |   |   |   |   |   |   |   |   |    |    |    |    |    |



Final Year Project 2

| Project Activities                                 | Week |   |   |   |   |   |   |   |   |    |    |    |    |    |
|--|------|---|---|---|---|---|---|---|---|----|----|----|----|----|
|  | 1    | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
| Project work                                       |      |   |   |   |   |   |   |   |   |    |    |    |    |    |
| Submission of Progress Report                      |      |   |   |   |   |   |   | ★ |   |    |    |    |    |    |
| Pre-SEDEX  |      |   |   |   |   |   |   |   |   |    | ★  |    |    |    |
| Submission of Draft Report                         |      |   |   |   |   |   |   |   |   |    |    | ★  |    |    |
| Submission of Dissertation                         |      |   |   |   |   |   |   |   |   |    |    |    | ★  |    |
| Submission of Technical Paper                      |      |   |   |   |   |   |   |   |   |    |    |    | ★  |    |
| Oral Presentation                                  |      |   |   |   |   |   |   |   |   |    |    |    |    | ★  |
| Submission of Project Dissertation<br>(Hard Bound) |      |   |   |   |   |   |   |   |   |    |    |    |    | ★  |

3.3 Simulation Tool



ANSYS FLUENT 14.0 is a CFD software package to simulate fluid flow problems. It uses the finite-volume method to solve the governing equations for a fluid. It provides the capability to use different physical models such as incompressible or compressible, inviscid or viscous, laminar or turbulent, etc.



## **CHAPTER 4**

### **RESULTS AND DISCUSSION**

#### **4.1 Dispersion Behavior of Fuel Gases in Enclosed Geometry**

In this section of study, we want to compare the mixing behavior of the fuel gases with air. At time  $t = 0$  s, the lower 10cm is filled with pure fuel gases while the other 90% of the geometry is filled with air. These gases are then released as time is started and let to mix with air that overlaying the fuel gases. Snapshot of mixing behavior of fuel gases are taken at certain time and will be compared. Technically, if the density difference between the fuel gases and air is greater, then the greater the mixing behavior will be.

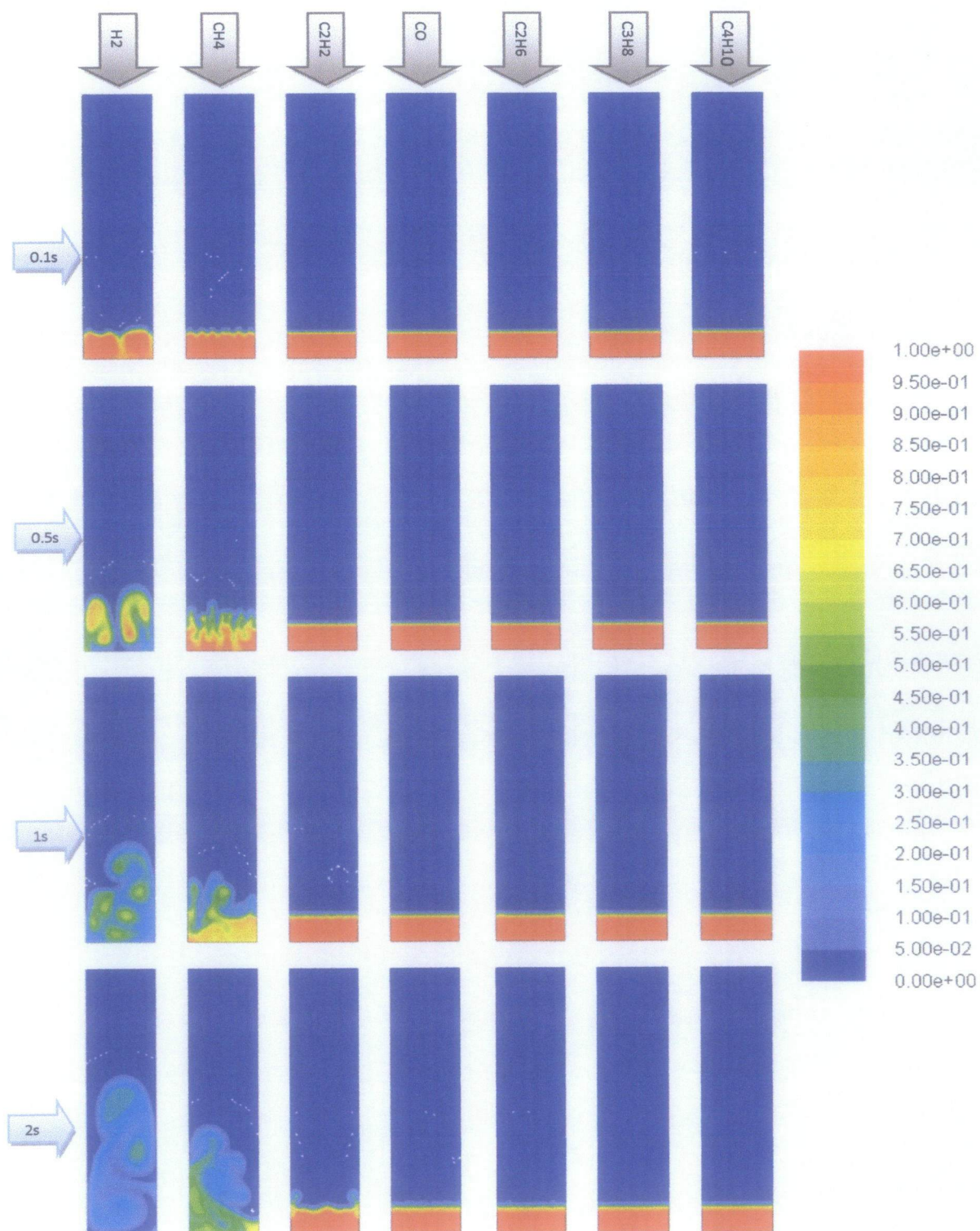


Figure 4.1 (a): Dispersion Behavior of Fuel Gases



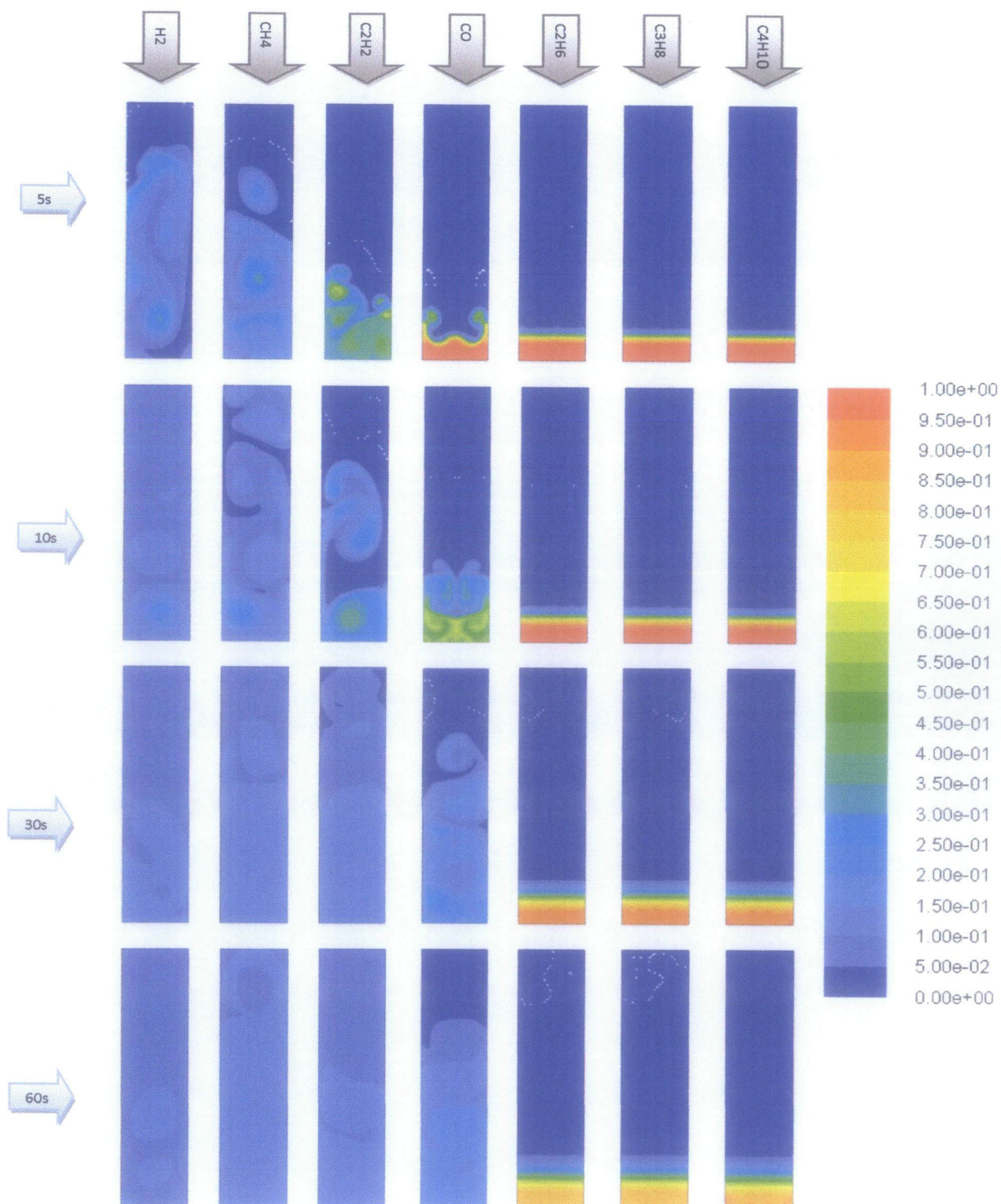


Figure 4.1 (b): Dispersion Behavior of Fuel Gases

Figure 4.1 (a) and 4.1 (b) shows the contour of mole fraction of each fuel gases at different times. The color of the contour must be referred to the scale to get the mole fraction of each fuel gas that disperses.

From figure 4.1 (a) at  $t= 0.1s$ , it can observed that hydrogen and methane already started to move upward while the other fuel gases still do not started to disperse. This shows that both of the gases have very high diffusion coefficient compared to other fuel gases. Apart from high diffusion coefficient, it also happen because there are large different between the density of hydrogen and methane when compared to the density of air.

Table 4.1: Density Comparison

| Fuel Gases      | Density<br>( $kg/m^3$ ) | Density Ratio (Density of Fuel Gas/Density of Air) |
|-----------------|-------------------------|--|
| Methane         | 0.668                   | 0.554  |
| Hydrogen        | 0.0899                  | 0.0746   |
| Ethane          | 1.264                   | 1.049  |
| Propane         | 1.882                   | 1.562  |
| Butane          | 2.489                   | 2.066  |
| Acetylene       | 1.092                   | 0.906  |
| Carbon Monoxide | 1.15                    | 0.92   |

At 2 seconds dispersion time, it can be seen that acetylene, carbon monoxide and ethane has also started to disperse. We can also see that hydrogen and methane still trying to move in axial direction of the geometry as less dense gas will always have a tendency to go higher. Then at  $t = 5s$ , mixing behavior can be seen for carbon monoxide.



After 60 seconds, it shows that heavy fuel gases namely ethane, propane and butane will stay at the bottom part of the geometry and will only disperse in radial direction. It is prove by the concentration decay of those gases. This shows that instead of buoyancy effects, the molecular differences between fuel gases and air play far more important role in dispersion of gases. Even after 60 seconds there is no obvious mixing behavior in the axial direction.

In order to obtain the time taken for the fuel gases to reach to the top, the following graphs were plotted.

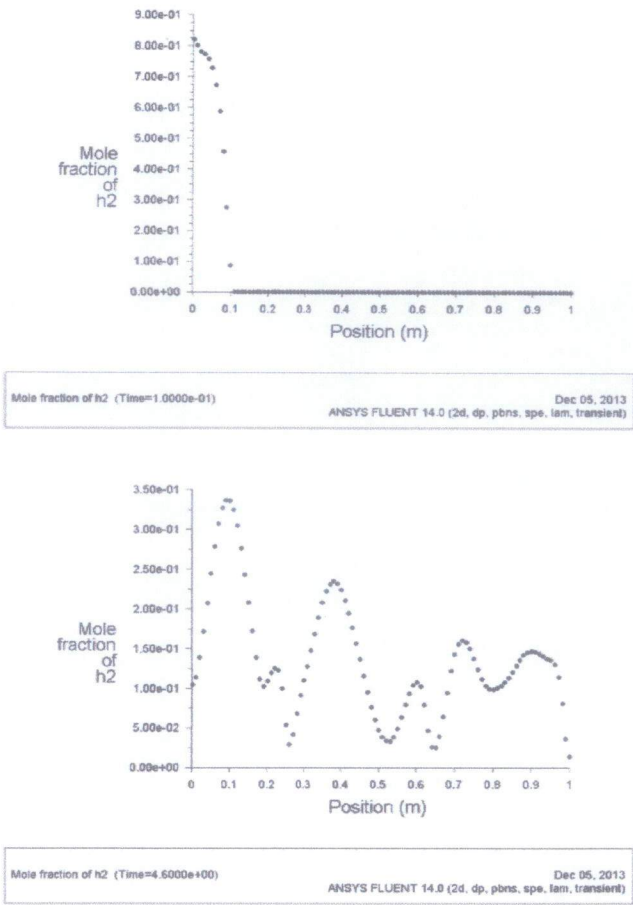


Figure 4.2: Graph of Mole Fraction of H<sub>2</sub> vs. Position along centre of Geometry

The graph shows the distribution of hydrogen mole fraction along centerline of the geometry at 0.1 seconds and at 4.6 seconds. When  $t = 0.1$  seconds, it can be seen that the

mole fraction of hydrogen at the bottom of the geometry (position = 0) has reduced to less than 0.8. This shows that part of the hydrogen has started to disperse in axial direction. At 4.6 seconds, it is the first time that mole fraction of hydrogen increase more than 0. This indicates that at 4.6 seconds, is the time where hydrogen reaches the top of the geometry.

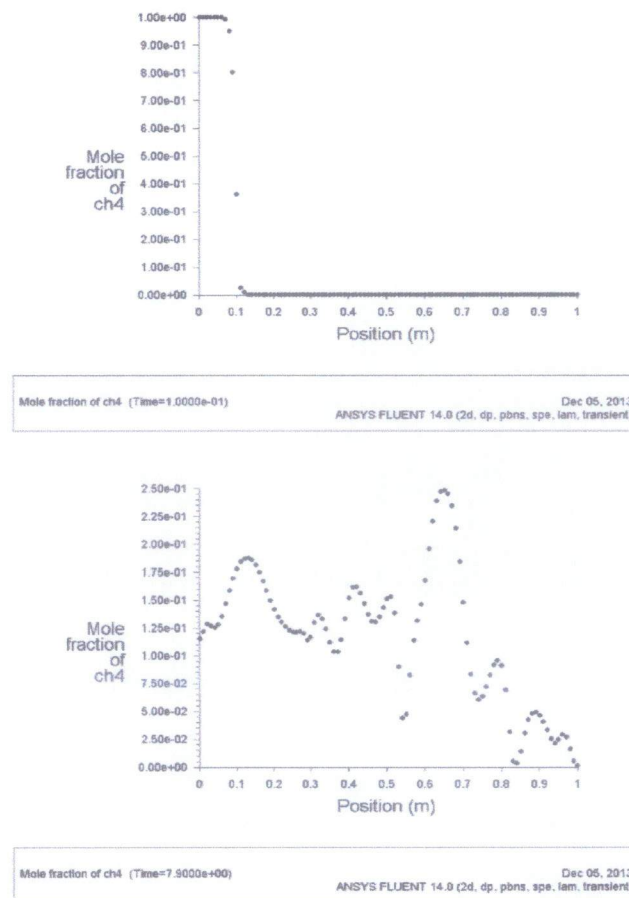


Figure 4.3: Graph of Mole Fraction of CH<sub>4</sub> vs. Position along centre of Geometry

For methane, the time for the gas to reach top of the geometry is 7.9 seconds. It can be compared that at 0.1 seconds that at the bottom of the geometry, the mole fraction of methane is still 1 which indicates that the mixing behavior is still slow.

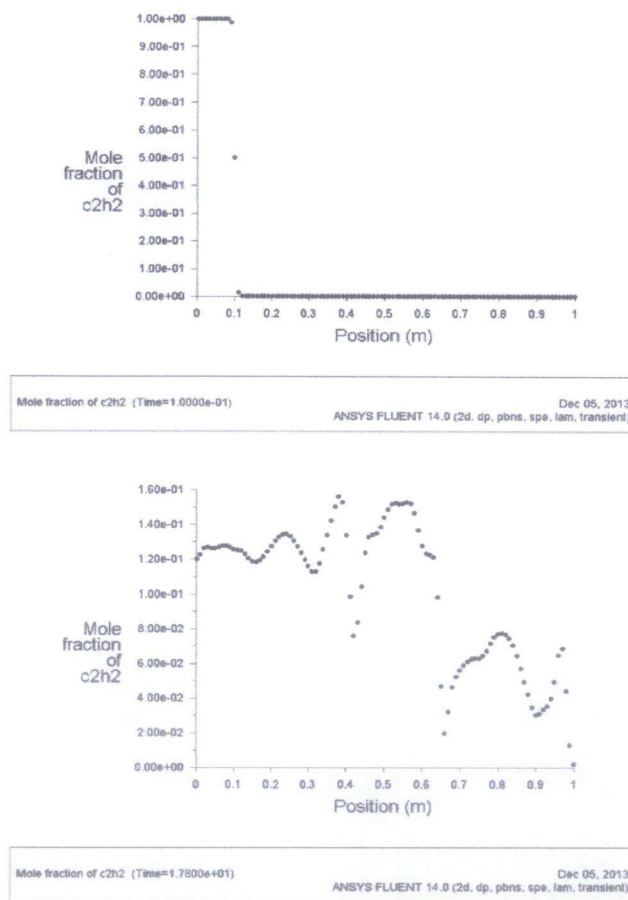


Figure 4.4: Graph of Mole Fraction of  $C_2H_2$  vs. Position along centre of Geometry

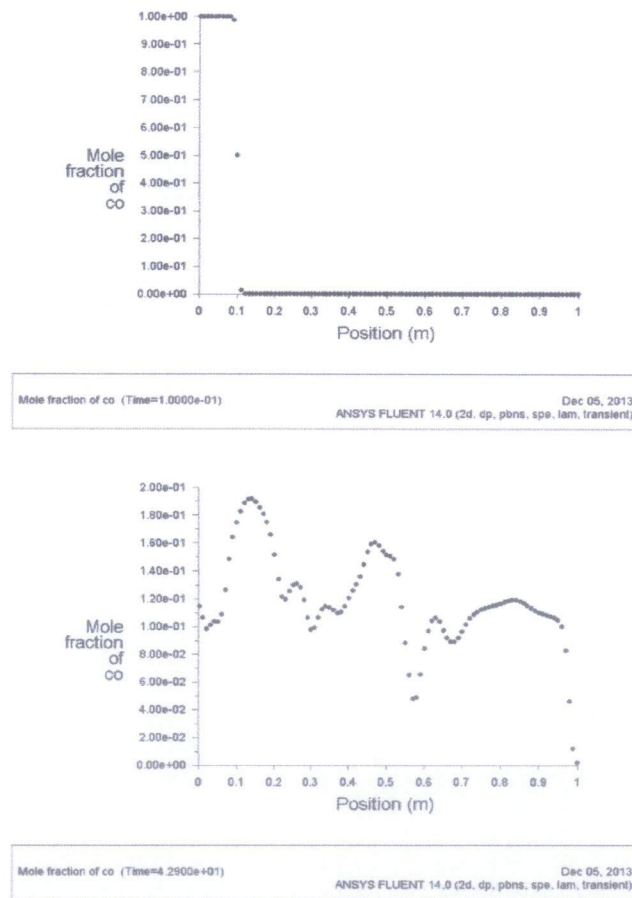


Figure 4.5: Graph of Mole Fraction of CO vs. Position along centre of Geometry

The time taken for acetylene and carbon monoxide to reach the top of geometry is 17.8 seconds and 42.9 seconds respectively. When compared to literature by Shravan & Umit which investigate the dispersion of hydrogen in the same geometry, the time taken for hydrogen gas to reach top is approximately the same with this project.



Table 4.2: Time Taken to Reach Top of Geometry

| Fuel Gas        | Time taken to reach top (s) |
|-----------------|-----------------------------|
| Hydrogen        | 4.6                         |
| Methane         | 7.9                         |
| Acetylene       | 17.8                        |
| Carbon Monoxide | 42.9                        |
| Ethane          | -                           |
| Propane         | -                           |
| Butane          | -                           |

So it can be concluded in this section that fuel gases that have density ratio more than 1 will stay at the bottom and disperse majorly in radial direction while fuel gases that has density ratio less than 1 will surely disperse through air and get to the top of the geometry. In addition of that, it proves that density difference has greater effect on dispersion compared to the buoyancy of the material in air.

#### 4.2 Formation of Flammability Region

Flammable region mark an area where the fuel gases will create fire even if there is tiny spark. The region is bounded by the upper flammability limit and lower flammability limit for each gas. Table below shows the range of concentration in which flammable region will form:

Table 4.3: Range of Flammability Region

| Fuel Gases       | Range of Flammable in % |
|------------------|-------------------------|
| By volume of air |                         |
| Methane          | 5 - 15                  |
| Hydrogen         | 4 - 75                  |
| Ethane           | 3 - 12.4                |
| Propane          | 2.1 - 10.1              |
| Butane           | 1.6 - 8.4               |
| Acetylene        | 2.5 - 82                |
| Carbon Monoxide  | 12 - 75                 |

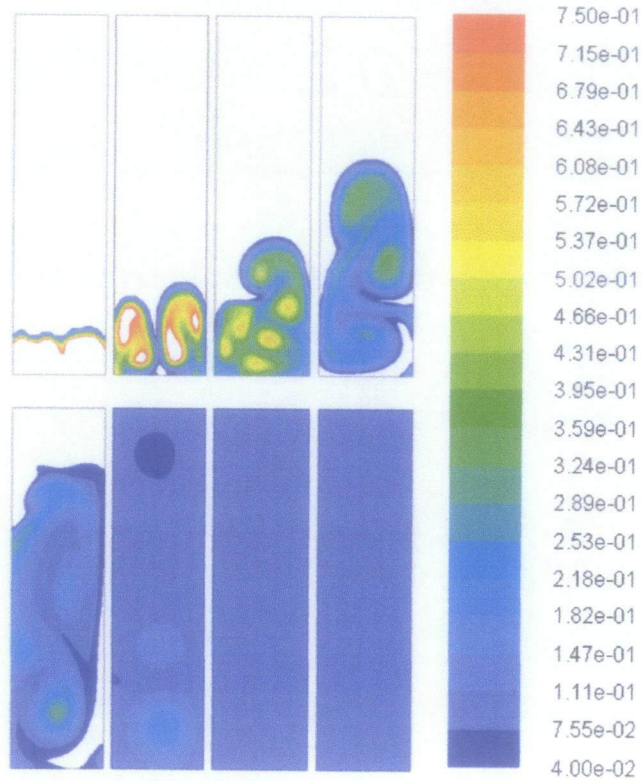


Figure 4.6: Formation of Flammability Region for Hydrogen

Figure 4.6 demonstrates how fast hydrogen will form flammable region. At  $t = 2s$ , the flammable region has already take up more than half of the container and as quick as 10 seconds, the geometry was completely prone to fire. In addition of that, this simulation was done without the effect of jet momentum and wind effects, which make the formation of flammable region in real life actually faster than the prediction of this simulation. Hydrogen also has the second widest range of flammability region next to acetylene which is 4-75 volume % in air.

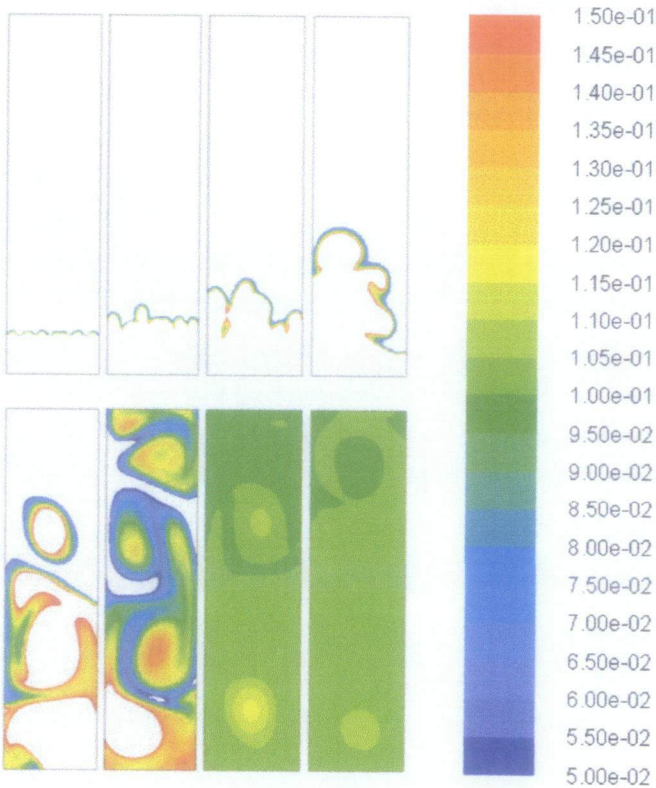


Figure 4.7: Formation of Flammability Region for Methane



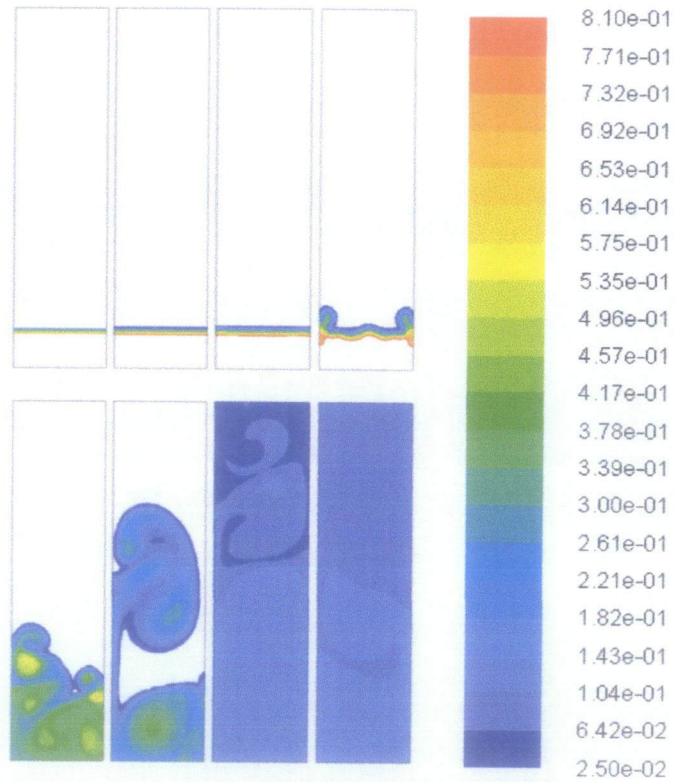


Figure 4.8: Formation of Flammability Region for Acetylene

Figure 4.7 and figure 4.8 shows the formation of flammability region of methane and acetylene respectively. Even the range of flammable region of methane is only 5-15 volume%, if compared with range of flammable region of acetylene which is wider, the formation of flammability region of methane is faster. If we compared both formation of flammability region at  $t = 5s$ , flammable region for methane already exceed half geometry where the flammability region for acetylene is only at quarter of geometry. This is because methane disperses faster than acetylene thus forming the flammability region faster.

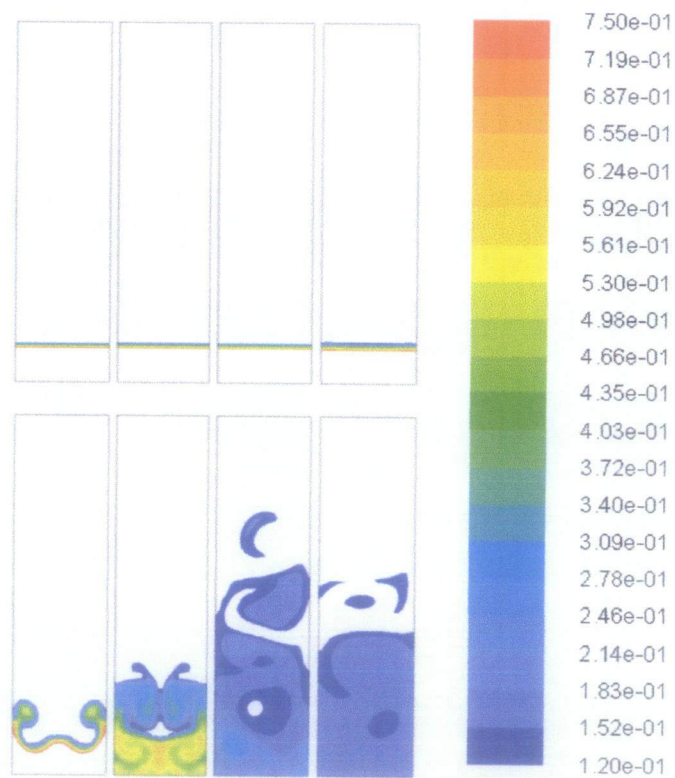


Figure 4.9: Formation of Flammability Region for Carbon Monoxide



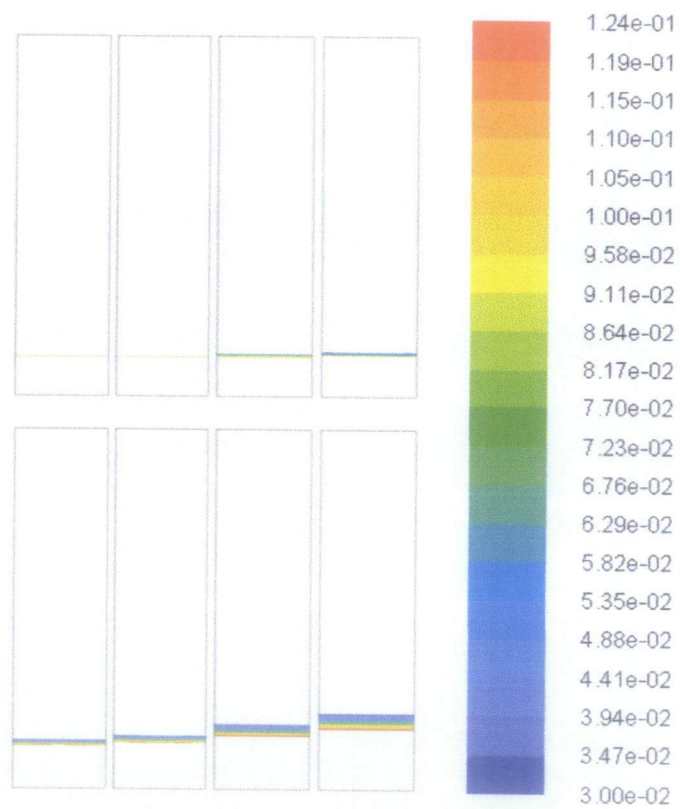


Figure 4.10: Formation of Flammability Region for Ethane

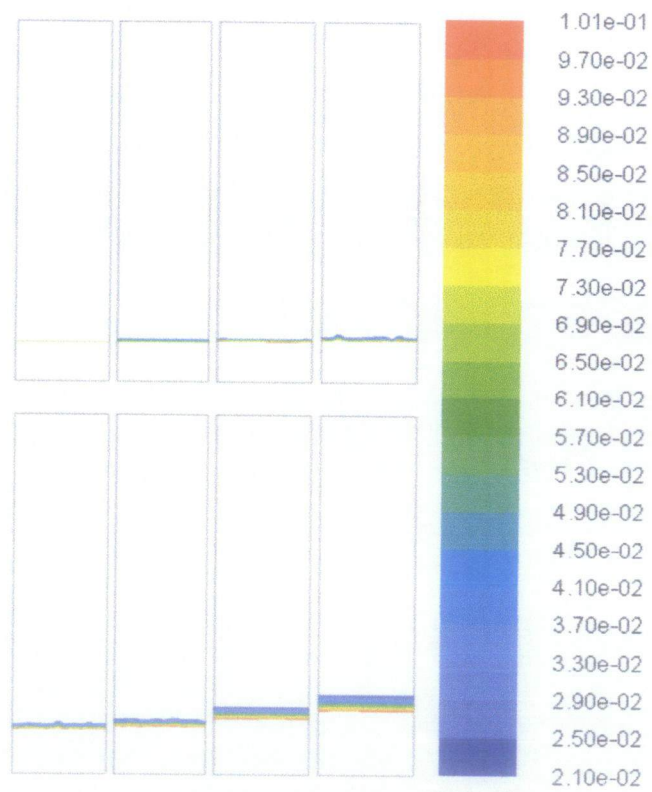


Figure 4.11: Formation of Flammability Region for Propane

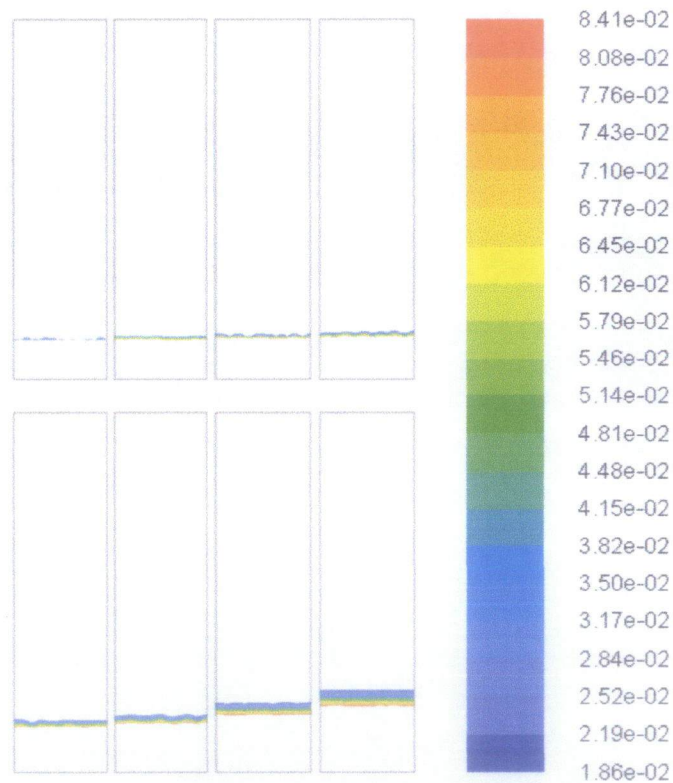


Figure 4.12: Formation of Flammability Region for Butane

As for heavy fuel gases (ethane, propane, and butane), the flammability region will stay around the part where the fuel gases started to mix with air. The flammability range of heavy fuel gases is quite limited compared to acetylene and hydrogen. With low dispersion and narrow range of flammability region, the heavy gas will of course poses less threat.

### 4.3 Comparison of Open Top Geometry and Enclosed Geometry

In this section, the dispersion behavior of fuel gases in open top geometry is compared with the dispersion behavior of fuel gases in enclosed geometry of the same dimension. After some simulation was done, difference can

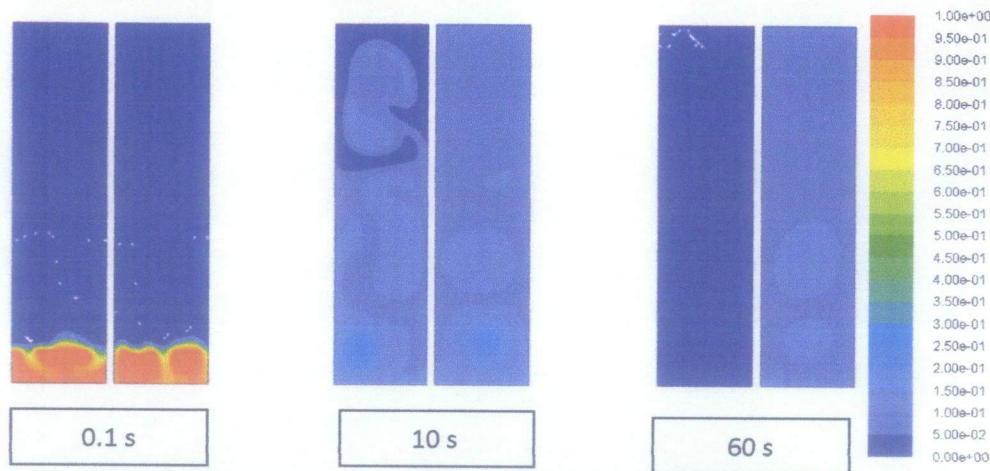


Figure 4.13: Comparison of dispersion behavior of hydrogen between open top geometry (left) and enclosed geometry (right)

From the result obtained, the difference in dispersion behavior between these two conditions is not much. Figure 4.13 suggests that in enclosed geometry, the dispersion will be faster. Also when observed at  $t = 60$  seconds, it clearly shows that most of the hydrogen has escape through the top leaving only small portion of it in the geometry for open top geometry. In contrast of that, at  $t = 60$  seconds for enclosed geometry, the concentration distribution seems to be evenly spread throughout the whole geometry.



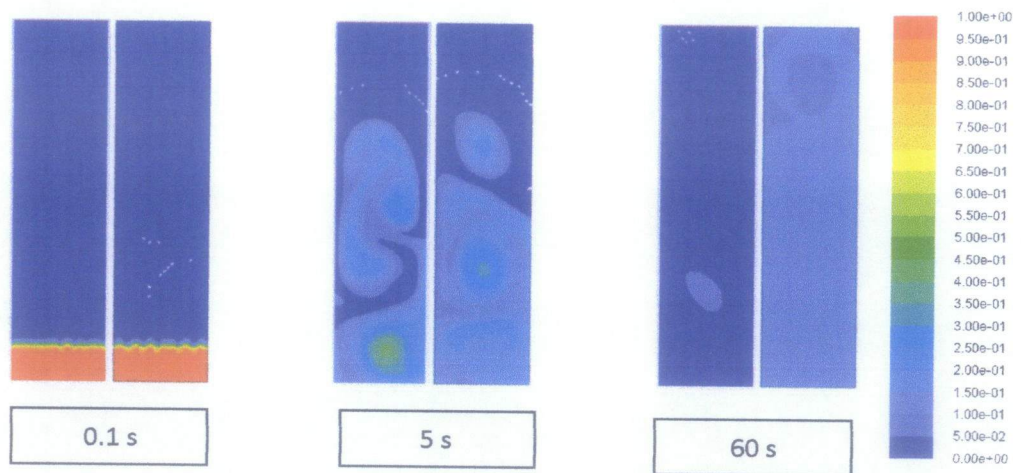


Figure 4.14: Comparison of dispersion behavior of methane between open top geometry (left) and enclosed geometry (right)

When the pressure is checked at the top of the geometry, there is 100 Pa difference between the inside of the geometry and outer pressure. So there is a little negative pressure gradient from top to bottom that suppress the gas from disperse to the top of the geometry.

## **CHAPTER 5**

### **CONCLUSION AND RECOMMENDATION**

As conclusion, this report discussed the fundamental findings on transient mixing of 7 different fuel gases namely hydrogen, methane, ethane, propane, butane, acetylene and carbon monoxide. The main focus is to compare the dispersion behavior of these gases and to compare the formation of flammability region. Apart from that, different geometry of open top and enclosed geometry are also being compared.

After comparison has been made, it is proven that the diffusion rate of gases is affected primarily by the density ratio or the density difference between air and fuel gases. Other factors that affect the dispersion are the molecular weight and the buoyancy effect of the gases itself. For the first analysis, it is recorded that hydrogen reaches the top of geometry fastest with just 4.6 seconds followed by methane, acetylene and carbon monoxide with the time 7.9 seconds, 17.8 seconds, and 42.9 seconds respectively. The other 3 fuel gases which are ethane, propane and butane did not make it to the top as each of them is heavier than air.

As for the second analysis which is the formation of flammability region, the data acquired is as predicted. The light fuel gases will occupy the whole geometry and form flammability region throughout the whole geometry while heavy fuel gases just tend to concentrate at the bottom of the geometry and form the flammability region along the mixing line. The formation time is affected by the range set by upper flammability limit (UFL) and lower flammability limits (LFL) and also affected by the dispersion rate of each fuel gases. Methane has much more narrower range of flammability region compared to acetylene. But it can be seen that methane form

flammability region faster compared to acetylene. This confirms that the formation of flammability region is affected by the range of flammable region and the dispersion rate of the fuel gases.

Last but not least, for recommendation, finer mesh should be used to increase the accuracy of results acquired. The time steps used also needed to be lower. In this study, the mesh and time steps used is quite high because to reduce the computing time. Also the geometry needed to be turned into more complicated geometry and done in 3D simulations. Other variables such as temperature, boiling and melting point of fuel gases, pressure of column should also be considered. Lastly, the usage of other software such as PHAST should also be considered.

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